Lattice determination of α_s in 3-flavour QCD

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ALPHA Collaboration

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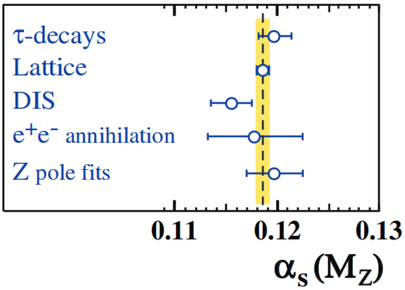
Currently quoted results for $\alpha_s(m_Z)$

World average [PDG 2014]: $\alpha_s(m_Z) = 0.1185(6)$



- PDG error estimate determined by lattice results! How realistic are these small errors?
- FLAG group average: $\alpha_s(m_Z)|_{\text{lattice}} = 0.1184(12)$ [arXiv:1310.8555v2]

ALPHA collaboration project

Build on CLS effort [Bruno et al, JHEP 1502 (2015) 043]:

- $N_\mathrm{f} = 2 + 1$ QCD
- nonperturbatively O(a) improved Wilson quarks & Lüscher-Weisz gauge action;
- open boundary conditions (avoids topology freezing)

Use 3 input parameters from experiment, e.g.

$$F_K, m_\pi, m_K \qquad \Rightarrow \qquad m_u = m_d, m_s, g_0$$

$\Rightarrow$ everything else becomes a prediction, for instance

$$\alpha_s^{(N_\mathrm{f}=3)}(100 \times F_K) \quad \text{(in any renormalization scheme)}$$

Final goal: $\alpha_s^{(N_\mathrm{f}=5)}(m_Z)$ in the $\overline{\mathrm{MS}}$-scheme

- Matching to $N_\mathrm{f} = 5$ across the charm and bottom thresholds
- Perturbative matching probably fine for bottom, unclear for charm (not discussed here).

The QCD Λ-parameter and $\alpha_s(\mu) = \bar{g}^2(\mu)/4\pi$

$$\Lambda = \mu\left[b_0\bar{g}^2(\mu)\right]^{-\frac{b_1}{2b_0^2}} \mathrm{e}^{-\frac{1}{2b_0\bar{g}^2(\mu)}} \exp\left\{-\int_0^{\bar{g}(\mu)} dg \left[\frac{1}{\beta(g)} + \frac{1}{b_0 g^3} - \frac{b_1}{b_0^2 g}\right]\right\}$$

- <u>exact</u> solution of Callan-Symanzik equation!
- Assume: coupling $\bar{g}(\mu)$ non-perturbatively defined, N_f massless quarks
- $\beta(g)$ has expansion $\beta(g) = -b_0 g^3 - b_1 g^5 + ..$

$$b_0 = (11 - \tfrac{2}{3}N_\mathrm{f})/(4\pi)^2, \qquad b_1 = (102 - \tfrac{38}{3}N_\mathrm{f})/(4\pi)^4, \quad \ldots$$

- Scheme dependence of Λ <u>almost</u> trivial:

$$g_\mathrm{X}^2(\mu) = g_\mathrm{Y}^2(\mu) + c_\mathrm{XY} g_\mathrm{Y}^4(\mu) + \ldots \quad \Rightarrow \quad \frac{\Lambda_\mathrm{X}}{\Lambda_\mathrm{Y}} = \mathrm{e}^{c_\mathrm{XY}/2b_0}$$

$\Rightarrow$ use $\Lambda_{\overline{\mathrm{MS}}} = \Lambda_\mathrm{QCD}$ as reference!

The QCD Λ-parameter and $\alpha_s(\mu) = \bar{g}^2(\mu)/4\pi$

$$\Lambda = \mu\left[b_0\bar{g}^2(\mu)\right]^{-\frac{b_1}{2b_0^2}} \mathrm{e}^{-\frac{1}{2b_0\bar{g}^2(\mu)}} \exp\left\{-\int_0^{\bar{g}(\mu)} dg\left[\frac{1}{\beta(g)} + \frac{1}{b_0 g^3} - \frac{b_1}{b_0^2 g}\right]\right\}$$

- Continuum relation, exact at any scale μ:
  - require large μ to evaluate integral perturbatively
  - require small μ to match hadronic scale

$\Rightarrow$ problem of large scale differences:

- The scale μ must reach the perturbative regime: $\mu \gg \Lambda_{\mathrm{QCD}}$
- The lattice cutoff must still be larger: $\mu \ll a^{-1}$
- The volume must be large enough to contain pions: $L \gg 1/m_\pi$
- Taken together a naive estimate gives

$$L/a \gg \mu L \gg m_\pi L \gg 1 \quad \Rightarrow L/a \simeq \mathrm{O}(10^3)$$

$\Rightarrow$ widely different scales cannot be resolved simultaneously on a single lattice!

Step scaling function

- Widely different scales cannot be resolved simultaneously on a *single* lattice

$\Rightarrow$ break calculation up in steps [Lüscher, Weisz, Wolff '91; Jansen et al. '95]:

1. define $\bar{g}^2(L)$ that runs with the space-time volume, i.e. $\mu = 1/L$
2. construct the step-scaling function

$$\sigma(u) = \bar{g}^2(2L)\Big|_{u=\bar{g}^2(L)}$$

   for a range of values $u \in [u_{\text{min}}, u_{\text{max}}]$
3. iteratively step up/down in scale by factors of 2:

$$\bar{g}^2(L_{\text{max}}) = u_{\text{max}} \equiv u_0, \quad u_k = \sigma(u_{k+1}) = \bar{g}^2(2^{-k}L_{\text{max}}), \quad k = 0, 1, \ldots$$

4. match to hadronic input at a hadronic scale L_{max}, i.e. $F_K L_{\mathrm{max}} = \mathrm{O}(1)$
5. once arrived in the perturbative regime extract Λ_{QCD}

Lattice approximants $\Sigma(u, a/L)$ for $\sigma(u)$

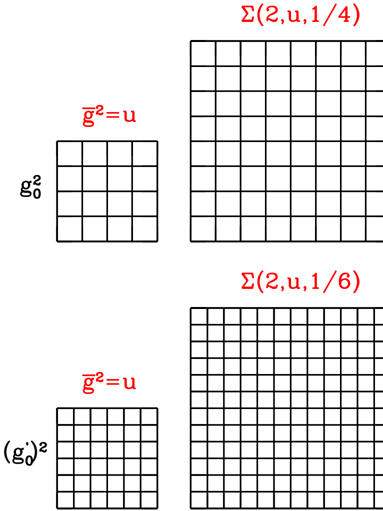
- choose g_0 and $L/a = 4$, measure $\bar{g}^2(L) = u$ (this sets the value of u)
- double the lattice and measure

$$\Sigma(u, 1/4) = \bar{g}^2(2L)$$

- now choose $L/a = 6$ and tune g_0' such that $\bar{g}^2(L) = u$ is satisfied
- double the lattice and measure

$$\Sigma(u, 1/6) = \bar{g}^2(2L)$$

- $\sigma(u) = \lim_{a/L \to 0} \Sigma(u, a/L)$.
- change u and repeat...



Wanted: renormalized finite volume coupling, which...

- is non-perturbatively defined in a finite space-time volume;
- can be expanded in perturbation theory (at least $\leq$ 2-loop) with reasonable effort;
- is gauge invariant;
- is quark mass-independent (defined in the chiral limit).
- can be evaluated by MC simulation with good statistical precision

$\Rightarrow$ not easy to satisfy! Here:

1. impose Schrödinger functional (SF) boundary conditions: periodic in space, Dirichlet in time
2. use 2 definitions of the coupling
   - traditional SF coupling [Narayanan et al. '92]
   - gradient flow coupling & SF b.c.'s [Fritsch & Ramos '13]

SF coupling

- (inhomogeneous) Dirichlet conditions for the gauge field

$\Rightarrow$ induce family of background gauge fields B_μ with parameter η.

- With some care the induced background fields are unique up to gauge equivalence.
- Effective action

$$\mathrm{e}^{-\Gamma[B]} = \int D[A, \psi, \overline{\psi}]\mathrm{e}^{-S[A,\psi,\overline{\psi}]}$$

- Perturbative expansion:

$$\Gamma[B] = \tfrac{1}{g_0^2}\Gamma_0[B] + \Gamma_1[B] + \mathrm{O}(g_0^2)$$

- Define

$$\frac{1}{\bar{g}_{\mathrm{SF}}^2(L)} = \frac{\partial_\eta \Gamma[B]}{\partial_\eta \Gamma_0[B]} = \frac{\langle \partial_\eta S \rangle}{\partial_\eta \Gamma_0[B]}$$

$\Rightarrow$ SF coupling is defined by the response of the system to a change of a colour electric background field. [Narayanan et al. '92]

Gradient flow & renormalized finite volume coupling

- QCD, gauge field $A_\mu(x)$, Yang-Mills gradient flow equation:

$$\partial_t B_\mu(t,x) \quad = \quad D_\nu G_{\nu\mu}(t,x) \quad \left(= -\frac{\delta S_g[B]}{\delta B_\mu(t,x)}\right), \quad B_\mu(0,x) = A_\mu(x)$$

  with field tensor $G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]$.

- Local gauge invariant composite fields at positive flow time $t > 0$ such as

$$E(t,x) = -\tfrac{1}{2}\,\mathrm{tr}\,\{G_{\mu\nu}(x,t)G_{\mu\nu}(x,t)\}$$

  are renormalized; no mixing with other fields of same or lower dimensions! [Lüscher & Weisz '2012];

- Explicit one-loop calculation (infinite volume, dimensional regularization) [Lüscher 2010]:

$$\langle E(t,x)\rangle = \frac{3g^2_{\overline{\mathrm{MS}}}(\mu)}{16\pi^2 t^2}\left(1 + \frac{1.0978 + 0.0075\,N_f}{4\pi} g^2_{\overline{\mathrm{MS}}}(\mu) + \ldots\right), \quad \mu = \frac{1}{\sqrt{8t}}$$

  $\Rightarrow$ $E(t,x)$ is, for $t > 0$, a renormalized field; unlike $E(0,x)$ which has a quartic and a logarithmic divergence!

Gradient flow couplings

- Infinite volume: Non-perturbative definition of a renormalized "gradient flow coupling" at scale $\mu = 1/\sqrt{8t}$:

$$g^2_{\mathrm{GF},\infty}(\mu) \stackrel{\mathrm{def}}{=} \frac{16\pi^2}{3} t^2 \langle E(t,x) \rangle$$

- Finite volume: consider $\langle E(t,x) \rangle$ in a finite box of dimension L^4, fix the ratio $c = \sqrt{8t}/L$ and define

$$\bar{g}^2_{\mathrm{GF}}(L) = \mathcal{N}(c)^{-1} t^2 \langle E(t,x) \rangle, \qquad \lim_{c \to 0} \mathcal{N}(c) = \frac{3}{16\pi^2}$$

- defines family of renormalized couplings, with parameter c. (typical range from 0.2 to 0.5);
- $\mathcal{N}(c)$ is calculable in lowest order perturbation theory; depends on b.c's for the gauge field; periodic in space; time direction:
  - periodic b.c.'s [Fodor et al. 2012]
  - $\Rightarrow$ SF (Dirichlet) b.c.'s [Fritzsch & Ramos 2012], <u>used here!</u>
  - twisted periodic b.c.'s [Ramos 2013]
  - open-SF (Neumann-Dirichlet) b.c.'s [Lüscher 2013]

Comparison g_{GF} vs. g_{SF}

SF-coupling:

- 3-loop β-function (i.e.b_2) is known [Bode, Weisz, Wolff '99]
- 2-loop c_t known: O(a) boundary effects highly suppressed
- $\Delta(1/\bar{g}^2) \propto (\Delta L)/L$, roughly independent of $\bar{g}$.
- requires very large statistics; variance increases with L/a.
- large physical volumes very difficult (N.B. coupling defined by variation of b.c.'s).

GF-coupling (finite volume, SF b.c.'s)

- high statistical precision
- can be measured in large physical volumes; ideal to match hadronic physics!
- $\Lambda_{\mathrm{GF}}/\Lambda_{\mathrm{QCD}}$ not yet known; only universal b_0, b_1 can be used.
- $\Delta(1/\bar{g}^2) \propto 1/\bar{g}^2$: more expensive as $\bar{g}$ decreases.
- Relatively large O(a^2) effects; can we reduce these?

Overview of the strategy

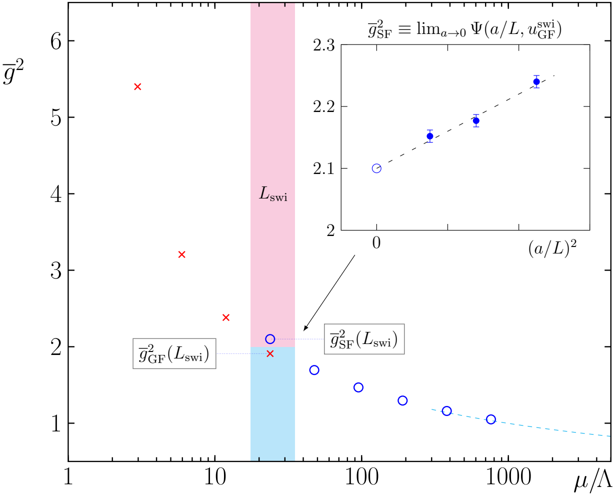
Combining the advantages of both couplings we proceed as follows:

- Compute the hadronic scale F_K on $N_\mathrm{f} = 2 + 1$ CLS configurations
- Compute $F_K \times L_\mathrm{max}$ (defined through the GF-coupling; aim for $L_\mathrm{max} \approx 0.5\mathrm{fm}$);
- Compute the step scaling functions for $\bar{g}^2_\mathrm{GF}(L)$;
- Perform 2-3 steps to cover the range from L_max to $L_\mathrm{swi} \approx 0.05\,\mathrm{fm}$
- At the intermediate scale L_swi switch from GF to SF scheme; also change from Lüscher-Weisz to Wilson gauge action;

$\Rightarrow$ obtain relation $L_\mathrm{swi}/L_\mathrm{max}$ and thus $L_\mathrm{swi} \times F_K$.

- Compute the step-scaling function for $\bar{g}^2_\mathrm{SF}(L)$
- extract $L_\mathrm{swi}\Lambda_\mathrm{QCD}$
- Combine results to obtain Λ_QCD/F_K

Overview of the strategy



(courtesy Patrick Fritzsch)

Computation of $L_{\mathrm{swi}}\Lambda_{\mathrm{QCD}}$

- Define L_{swi} implicitly by $\bar{g}^2_{\mathrm{SF}}(L_{\mathrm{swi}}) = 2.012$
- Obtain <u>continuum</u> step scaling function (SSF) by fit ansatz for continuum & cutoff effects

$$\sigma(u) = \bar{g}^2_{\mathrm{SF}}(2L)|_{u=\bar{g}^2_{\mathrm{SF}}(L)}$$

  for a range of u-values, $u \in [1.10891, 2.0120]$
- Given $\sigma(u)$ start with $u_0 = 2.012$ and find u_1, u_2,...,u_5.

$$u_{n-1} = \sigma(u_n), \quad n = 1, \ldots, 5, \qquad \Rightarrow \qquad u_n = \bar{g}^2_{\mathrm{SF}}\left(2^{-n} L_{\mathrm{swi}}\right)$$

- At scale $2^{-n} L_{\mathrm{swi}}$ obtain $L_{\mathrm{swi}}\Lambda_{\mathrm{SF}}$

$$L_{\mathrm{swi}}\Lambda_{\mathrm{SF}} = 2^n \left[b_0 u_n\right]^{-\frac{b_1}{2b_0^2}} \mathrm{e}^{-\frac{1}{2b_0 u_n}} \exp\left\{\frac{b_1^2 - b_2 b_0}{2b_0^3} u_n + \mathrm{O}(u_n^2)\right\}$$

- Connect to $\overline{\mathrm{MS}}$ scheme $\Lambda^{N_\mathrm{f}=3}_{\mathrm{SF}}/\Lambda^{N_\mathrm{f}=3}_{\mathrm{QCD}} = 0.382863(1)$

Simulations

- On lattices with sizes $L/a = 4, 6, 8, 12$ measure $u = \bar{g}^2(L)$.
- requires precise knowledge of massless limit, i.e. $\kappa_{\rm cr}(g_0, L/a)$
- Double lattice size and measure $\Sigma(u, a/L) = \bar{g}^2(2L)$
- analyze $\Sigma(u, a/L)$ directly
- Alternatively, reduce cutoff effects perturbatively up to 2-loop order:

$$\delta(u, a/L) = \frac{\Sigma(u, a/L) - \sigma(u)}{\sigma(u)} = \delta_1(L/a)u + \delta_2(L/a)u^2 + \mathrm{O}(u^3)$$

$\delta_{1,2}(L/a)$ are known [Bode, Weisz & Wolff '99]

$\Rightarrow$ cutoff effects in

$$\Sigma'(u, a/L) = \frac{\Sigma(u, a/L)}{1 + \delta_1(L/a)u + \delta_2(L/a)u^2}$$

start at order u^4!

Obtaining the SSF in the continuum

Example for global fit ansatz:

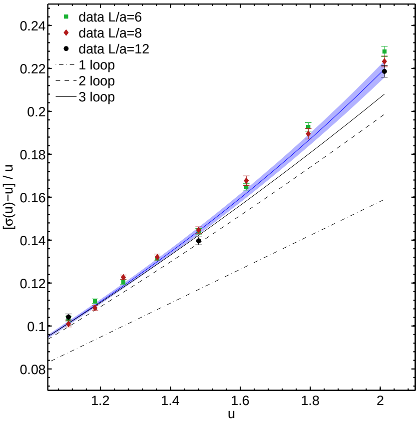
$$\Sigma'(u, a/L) = u + s_0 u^2 + s_1 u^3 + c_1 u^4 + c_2 u^5 + \rho_1 u^4 \frac{a^2}{L^2}$$

- s_0, s_1 fixed to perturbative values:

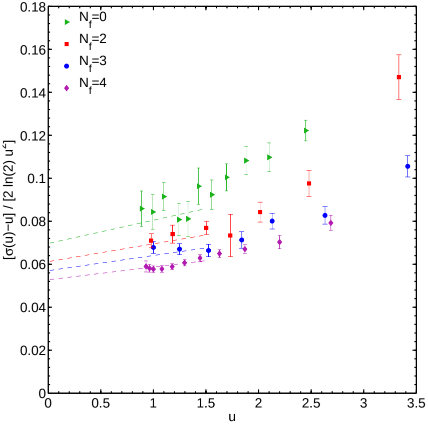
$$s_0 = 2b_0 \ln 2, \quad s_1 = s_0^2 + 2b_1 \ln 2$$

- 3 parameters: c_1, c_2, ρ_1; 19 data points,

$$\chi^2/\text{d.o.f.} = 1.099$$

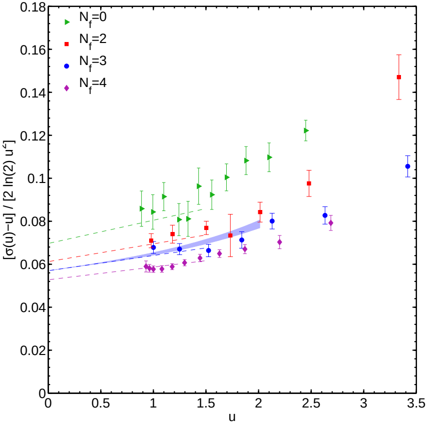


Precision compared to earlier results for $N_f = 0, 2, 3, 4$



- $N_f = 0, 2, 4$ [ALPHA,'92–'12]
- $N_f = 3$ [PACS-CS '09]

Precision compared to earlier results for $N_\mathrm{f} = 0, 2, 3, 4$



- $N_\mathrm{f} = 0, 2, 3, 4$ [ALPHA,'92–'15]
- $N_\mathrm{f} = 3$ [PACS-CS '09]
- Various fits (3-5 parameters, perturbatively improved & unimproved data), find stability after $n = 2, 3$ step-scaling steps

$$\Rightarrow L_\mathrm{swi}\Lambda_{\overline{\mathrm{MS}}}^{N_\mathrm{f}=3} = 0.0802(16)$$

(preliminary)

More details on the definition of g^2_{GF}

- Choose same bare action as CLS in large volume;
- SF boundaries: use variant B by [Aoki, Frezzotti, Weisz, '98]
- Boundary O(a) improvement: $c_{\mathrm{t}}, \tilde{c}_{\mathrm{t}}$ to 1-loop order [Aoki, Ide, Takeda '03; Vilaseca '15]
- Study of O(a) boundary effects (PT and quenched):
  1. $T = L$, $c = \sqrt{8t}/L = 0.3$ seems OK;
  2. advantageous to restrict to magnetic components at $x_0 = T/2$:

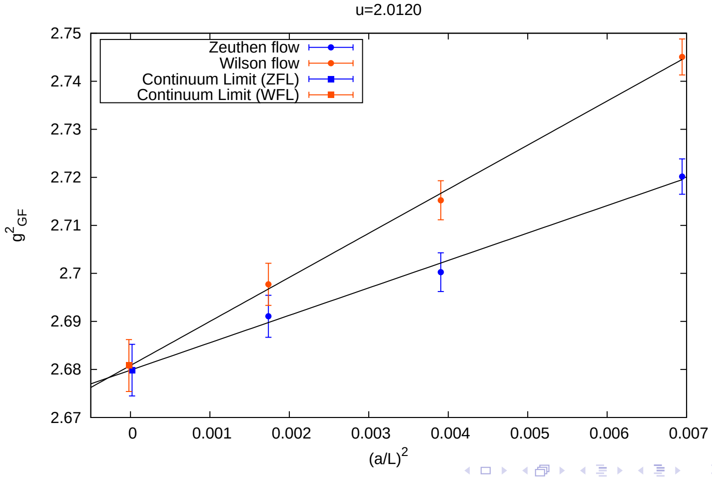
$$-\tfrac{1}{2}\langle \mathrm{tr}\,\{G_{kl}(t,x)G_{kl}(t,x)\}\rangle\big|_{x_0=T/2,T=L,m_{\mathrm{q}}=0} = \mathcal{N}(c,a/L)\,g^2_{\mathrm{GF}}(L)$$

- Use $\mathcal{N}(c,a/L)$ for given $L/a \Rightarrow g^2_{\mathrm{GF}} = g^2_0$ exact at tree-level.
- Wilson flow & O(a^2) improved Zeuthen flow
- Clover & O(a^2) improved observable
- topology freezing: use projection on $Q = 0$ sector [Fritzsch, Ramos, Stollenwerk '13]; becomes relevant for $L > 0.25$ fm

Matching at the switching scale $L_{\rm swi}$ (Wilson action)

$$\bar{g}^2_{\rm SF}(L_{\rm swi}) = 2.012 \Rightarrow (\beta, L/a) \to (\beta, 2L/a) \Rightarrow \bar{g}^2_{\rm GF}(2L_{\rm swi}) = 2.6808(54)$$

(preliminary)



Summary status: $\Lambda_{\mathrm{QCD}}^{N_\mathrm{f}=3}$ with target error $<$ 4-5%

- SF coupling for $L < L_{\mathrm{swi}} \approx 0.05\,\mathrm{fm}$;
  unprecedented precision (high statistics & precise tuning of κ):

$$\bar{g}^2_{\mathrm{SF}}(L_{\mathrm{swi}}) = 2.012 \quad \Rightarrow \quad L_{\mathrm{swi}}\Lambda_{\overline{\mathrm{MS}}}^{N_\mathrm{f}=3} = 0.0802(16) \quad (\text{preliminary})$$

- Definition of gradient flow coupling $\bar{g}^2_{\mathrm{GF}}(L)$ settled:
  - reduced boundary $\mathrm{O}(a)$ effects by restricting $E(t,x)$ to magnetic components;
  - Symanzik $\mathrm{O}(a^2)$ improvement: Zeuthen flow and observable.
- Matching at switching scale L_{swi}

$$\bar{g}^2_{\mathrm{GF}}(2L_{\mathrm{swi}}) = 2.6808(54) \quad (\text{preliminary})$$

- Running of $\bar{g}^2_{\mathrm{GF}}(L)$ from $0.05 - 0.1\,\mathrm{fm}$ to $0.5\,\mathrm{fm}$:
  - precision tuning of κ finished;
  - simulations for step scaling function underway.
- Connect to F_K on CLS config's: details to be defined.